

## Claims

1. A molecular stereochemical coding method for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule, said method comprising:

a hierarchy classifying step of assigning a start atom, which is to be noticed, to a zero-th hierarchy serving as the lowest hierarchy, assigning an atom, which is combined with said start atom on a higher hierarchy side, to a first hierarchy, assigning an atom, which is combined with said atom assigned to said first hierarchy, to a second hierarchy, and similarly, sequentially assigning atoms to hierarchies until the final hierarchy which is set so as to be specially requested;

a molecular tree forming step of setting a predetermined precedence rule for placing a plurality of atoms, which belong to the same hierarchy, in the order, and placing said atoms, which belong the same hierarchy, in the order every hierarchy in accordance with said precedence rule, to form a molecular tree every said start atom from a lower hierarchy to a higher hierarchy so as to express a bonding relationship between said plurality of atoms;

a coding step of noticing one of atoms, which are assigned to the  $(n+3)$ -th hierarchy, with respect to each of integers  $n$  assuming that  $n$  is an integer of 0 or more, in said molecular tree, deriving a dihedral angle between a plane, which is formed by an atom in the  $(n+3)$ -th hierarchy, an atom in the  $(n+2)$ -th hierarchy and an atom in the  $(n+1)$ -th hierarchy, and a plane, which is formed by the atom in the  $(n+2)$ -th hierarchy, the atom in the  $(n+1)$ -th hierarchy and an atom in the  $n$ -th hierarchy, with respect to a group comprising four atoms which consists of the noticed atom in the  $(n+3)$ -th hierarchy, the atom in the  $(n+2)$ -th hierarchy which is combined with the atom in the  $(n+3)$ -th hierarchy, the atom in the  $(n+1)$ -th hierarchy which is combined with the atom in the  $(n+2)$ -th hierarchy, and the atom in the  $n$ -th hierarchy which is combined with the atom in the  $(n+1)$ -th hierarchy, replacing the derived dihedral angle into an angular symbol, which is defined in accordance with a predetermined angle

setting a predetermined linear notation rule for expressing said molecular tree by a row of characters, carrying out the linear notation of a set of said plurality of angular symbols in accordance with said predetermined linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms.

wherein said configuration code preparing step causes an atom, which is to be noticed in the  $n$ -th hierarchy, to be positioned at a reference position in said angle dividing rule, integrally rotates all of said atoms belonging to the  $(n+3)$ -th hierarchy around a bonding axis, which connects the atom in the  $(n+1)$ -th hierarchy to the atom in the  $(n+2)$ -th hierarchy, so that an atom, which has a predetermined precedence in accordance with said precedence rule among said atoms belonging to the  $(n+3)$ -th hierarchy, is positioned at a predetermined angular position with respect to said reference position, gives an angular symbol according to said angle dividing rule to each of said atoms belonging to the  $(n+3)$ -th hierarchy, in accordance with an angular position after rotation with respect to said reference position, carries out the linear notation of a set of said plurality of angular symbols in accordance with said predetermined linear notation rule so as to correspond to said molecular tree, and prepares a configuration code for every said start atom.

wherein said planar structure code preparing step expresses said molecular tree by a set of planar structure symbols which planar-structurally express a bonding relationship between said plurality of atoms, carries out the linear notation of said set of planar structure symbols in accordance with said predetermined linear notation rule so as to correspond to said molecular tree, prepares a planar structure code indicative of the planar structure of the molecule with respect to said start atom, and similarly, prepares planar structure codes with respect to other start atoms.

5. A molecular stereochemical coding method as set forth in claim 2, wherein when it is impossible to rotate said atoms belonging to the (n+3)-th hierarchy around the bonding axis connecting the atom belonging to the (n+1)-th hierarchy to the atom belonging to the (n+2)-th hierarchy, said angular symbols given at said coding step are adopted as they are, and the linear notation of a set of said plurality of angular symbols is carried out in accordance with said predetermined linear notation rule so as to correspond to said molecular tree, to prepare said configuration codes for every said start atom.

7. A molecular stereochemical coding method as set forth in claim 1, wherein said precedence rule is a CANOST code precedence

rule.

8. A molecular stereochemical coding method as set forth in claim 1, wherein said predetermined linear notation rule is a CANOST code linear notation rule.

9. A molecular stereochemical coding method as set forth in claim 1, wherein at said molecular tree forming step, a group of atoms having a low degree of notice in the identification of stereochemistry are replaced with predetermined symbols to be masked.

10. A molecular stereochemical coding method as set forth in claim 1, wherein said predetermined angle dividing rule divides an angle of 360 degrees into a predetermined number of clock-dial-like angular ranges, and the divided angular ranges are reflected in the level of abundance to be unequally divided.

11. A molecular stereochemical coding method as set forth in claim 1, wherein at said conformation code preparing step, said conformation codes are prepared with respect to at least two of said start atoms, the hierarchy numbers of which are spaced from each other by three hierarchies or more.

12. A computer readable recording media, in which a program for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule has been recorded, said program comprising:

a hierarchy classifying step of assigning a start atom, which is to be noticed, to a zero-th hierarchy, assigning an atom, which is combined with said start atom on a higher hierarchy side, to a first hierarchy, assigning an atom, which is combined with said atom assigned to said first hierarchy, to a second hierarchy, and similarly, sequentially assigning atoms to hierarchies until the final hierarchy which is set so as to be specially requested;

a molecular tree forming step of setting a predetermined precedence rule for placing a plurality of atoms, which belong

00057510-050004  
1000000-075000

a coding step of noticing one of atoms, which are assigned to the  $(n+3)$ -th hierarchy, with respect to each of integers  $n$  assuming that  $n$  is an integer of 0 or more, in said molecular tree, deriving a dihedral angle between a plane, which is formed by an atom in the  $(n+3)$ -th hierarchy, an atom in the  $(n+2)$ -th hierarchy and an atom in the  $(n+1)$ -th hierarchy, and a plane, which is formed by the atom in the  $(n+2)$ -th hierarchy, the atom in the  $(n+1)$ -th hierarchy and an atom in the  $n$ -th hierarchy, with respect to a group comprising four atoms which consists of the noticed atom in the  $(n+3)$ -th hierarchy, the atom in the  $(n+2)$ -th hierarchy which is combined with the atom in the  $(n+3)$ -th hierarchy, the atom in the  $(n+1)$ -th hierarchy which is combined with the atom in the  $(n+2)$ -th hierarchy, and the atom in the  $n$ -th hierarchy which is combined with the atom in the  $(n+1)$ -th hierarchy, replacing the derived dihedral angle into an angular symbol, which is defined in accordance with a predetermined angle dividing rule, in accordance with the magnitude of the dihedral angle, giving the replaced angular symbol to the noticed atom in the  $(n+3)$ -th hierarchy, and similarly, giving angular symbols in accordance with the magnitudes of the dihedral angles with respect to other atoms to be noticed; and

setting a predetermined linear notation rule for expressing said molecular tree by a row of characters, carrying out the linear notation of a set of said plurality of angular symbols in accordance with said predetermined linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms.